

Curriculum Vitae

Bertil HALLE

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Academic degrees and positions

1998 –	Chair professor, Physical chemistry	Lund University, Technical faculty
1989 – 95	Senior scientist	Swedish Research Council
1986	Docent, Physical chemistry	Lund University
1982 – 84	Postdoctoral fellow	Dept of Applied Mathematics, Institute of Advanced Studies, Australian National University
1981	Ph D (Tekn Dr), Physical chemistry	Lund University

Commissions of trust (since 2000)

2010 –	Editorial Board	Journal of Chemical Physics
2009 –	Head	Dept of Biophysical Chemistry, Lund University
2009 –	Member	National Committee for Molecular Biosciences
2007	Study Section	Swedish Research Council
2005 –	Governing Council	International Society of Magnetic Resonance
2002 –	Advisory Subcommittee	IUPAC, Physical & Biophysical Chemistry Division
2003 – 2005	Research Board	Center for Chemistry and Chemical Engineering
1999 – 2005	Head	Dept of Biophysical Chemistry, Lund University
2000 – 2002	Governing Board	Center for Chemistry and Chemical Engineering
2000 – 2002	Undergraduate Board	Biotechnology and Chemical Engineering, LU
2001	Program Chairman	9 th Chianti Workshop on Magnetic Resonance
2000	Program Co-Chairman	1 st Sino-Swedish Symposium on Magnetic Resonance

Ph D students (principal supervisor)

2012 –	Filip Persson	1997 – 2003	Michael Gottschalk
2011 –	Zhiwei Chang	1993 – 1998	Haukur Jóhannesson
2007 – 2012	Johan Qvist	1992 – 1997	Stefan Gustafsson
2005 – 2009	Erik Persson Sunde	1989 – 1992	Ping Huang
2003 – 2008	Monika Davidovic	1986 – 1991	Per-Ola Quist
1998 – 2003	Kristofer Modig	1983 – 1988	Göran Carlström

Postdoctoral fellows

2011 –	Shuji Kaieda	Inst for Protein Res	Osaka Univ	Japan
2006 – 07	Carlos Mattea	NMR Group	Univ of Ulm	Germany
2002 – 04	Karim Snoussi	Groupe Biophysique	École Polytechnique, Palaiseau	France
2002 – 04	Fabian Vaca Chávez	Dept of Physics	Cordoba Univ	Argentina
2002 – 03	Flaminia C. Marincola	Dept of Chemistry	Cagliari Univ	Italy
2001 – 03	Tomas Nilsson	Dept of Phys Chem	Stockholm Univ	Sweden
1995 – 97	Kandadai Venu	Dept of Physics	Univ of Hyderabad	India
1993 – 95	Vladimir Denisov	Dept of Physics	Moscow State Univ	Russia
1987 – 89	István Furó	Ctr Res Inst Physics	Budapest	Hungary

Plenary lectures (selection)

2012	Gordon Research Conference on Biopolymers	Newport, US
2010	Gordon Research Conference on Water and Aqueous Solutions	Holderness, US
2010	KVA Symposium: Protein Biophysics in the Cell	Stockholm, SE
2009	Gordon Research Conference on Proteins	Holderness, US
2009	Euromar Magnetic Resonance Conference	Göteborg, SE
2009	6 th Conference on Fast Field-Cycling Relaxometry	Torino, IT
2008	Workshop on Water at Biological Interfaces	Hangzhou, CN
2008	Faraday Discussions 141: Water – From Interfaces to the Bulk	Edinburgh, UK
2008	Gordon Research Conference on Biomolecular NMR	Il Ciocco, IT
2007	ESF Conference on Water at Interfaces	Obergurgl, AU
2006	4 th Conference on Fast Field-Cycling Relaxometry	Torino, IT
2004	Gordon Research Conference on Water and Aqueous Solutions	Holderness, US
2004	Symposium on Water and Biomolecules	Osaka, JP
2003	Royal Society Discussion Meeting: The Molecular Basis of Life	London, UK
2001	Keystone Symposium on Frontiers of NMR Molecular Biology	Big Sky, US
1999	Telluride Workshop on Protein Dynamics	Telluride, US
1998	39 th Experimental NMR Conference	Asilomar, US
1998	Gordon Research Conference on Water and Aqueous Solutions	Holderness, US

Career summary

Bertil Halle received a MSc in Engineering Chemistry in 1977 from Lund University, spent one year at the University of California, and obtained his PhD in Physical Chemistry in Lund in 1981. Following a two-year Postdoctoral Fellowship at the Department of Applied Mathematics in the Institute of Advanced Studies of the Australian National University, he established his research group in Lund in 1984. He was appointed Associate Professor (Docent) in 1986; from 1989 to 1995 he held a Senior Researcher position funded by the Swedish Research Council; and in 1998 he was appointed (in competition with 27 candidates from 6 countries) to the Chair Professorship of Physical Chemistry at the Technical Faculty of Lund University, where he currently acts as Head of the Department of Biophysical Chemistry.

Research in the Halle group has always been highly multidisciplinary. Experimental as well as theoretical methods are developed and used to address central biological and biomedical problems from a molecular perspective. The focus is on the generic properties of molecular systems with far-reaching implications for fundamental understanding as well as biomedical utility. The investigated systems range in complexity from pure water (already a complex system!) – via proteins, nucleic acids and membranes – to colloidal systems, bacteria and spores. The PhD students and postdocs in the group frequently have a physics background, while collaborations with biochemists and microbiologists provide the specific competence needed to handle delicate biological systems. Most of the research carried out by the group is problem-driven, and virtually all of the group's publications describe research planned, executed and written up within the group. Despite its relatively small size, the Halle group had accumulated 6000 citations by March 2012 (ISI).

The Halle group is internationally recognized for their contributions in the areas of water science, protein biophysics and nuclear magnetic relaxation. The group has developed an NMR technique, Magnetic Relaxation Dispersion (MRD), that makes it possible to study how proteins and other biomolecules interact with, and are affected by, water, ions and other molecules in their physiological environment. This interaction is crucial for virtually all biological structures and processes, but the details are only now beginning to emerge. The Halle group plays a leading role in this rapidly expanding research field. Apart from its unique MRD laboratory assembled over the past decade, the group applies or develops X-ray crystallography, femtosecond fluorescence spectroscopy, quasielastic neutron scattering, statistical-mechanical modeling and computer simulations.

The Halle group is funded mainly by project grants from the Swedish Research Council and equipment grants from the K & A Wallenberg and Crafoord Foundations. In the three applications rounds in 2002, 2005 and 2008, the group received the largest (2002 & 2008) or second largest (2005) project grant awarded by the Swedish Research Council in the Natural and Engineering Sciences. The group's research has considerable potential for biomedical application. Examples include development of new methods for magnetic resonance imaging of soft tissue, for improved design of protein-targeting drugs, for intervention in protein misfolding diseases, and for endospore control in the food industry. Because of funding limitations, the group has so far not been able to pursue these exciting avenues in a systematic way.

Principal research accomplishments

- developed magnetic relaxation dispersion (MRD) into a quantitative tool for studies of biomolecule-solvent interactions and dynamics *in vitro* and *in vivo*
- established the highly dynamic nature of protein-water interfaces, with important implications for protein dynamics, folding, recognition and stability
- revealed structural and functional roles of internal water molecules in many proteins
- developed and applied new MRD-based techniques for studying protein dynamics, protein aggregation and protein folding
- provided the first experimental proof of ion penetration into the minor groove of the DNA double helix in solution
- resolved the long-standing cell-water controversy by using the MRD technique to observe single-water-molecule dynamics in living bacterial cells
- provided radically new insights about water and protein dynamics in bacterial spores and their role for spore resistance and dormancy
- elucidated the molecular basis of endogenous contrast in magnetic resonance images of soft tissue, including ^1H magnetic relaxation and ^1H - ^{14}N cross-relaxation
- contributed extensively to the theory of nuclear spin relaxation in biological and colloidal systems
- made theoretical and methodological contributions to protein crystallography, fluorescence spectroscopy and quasielastic neutron scattering
- developed and applied NMR spectroscopy and relaxation for probing the structure and dynamics of amphiphilic liquid crystals and other soft materials
- made pioneering studies of hydrogen bonding and proton transfer in liquid water
- demonstrated and characterized the jump-like translational and rotational molecular motion in liquid water using neutron scattering, NMR and MD simulations

Distinctions

2002-08	Largest or second-largest 3-year project grant in Sweden from VR-NT*
2002	"Excellent Researcher" award by the Swedish Research Council (as one among 21 PIs in Sweden within all branches of science, technology and medicine)
2000	One among 3 PIs in Sweden who received the highest ranking in the Swedish Research Council's international evaluation of Swedish physical chemistry groups
1986 -	Declined all personal prizes and awards (excluding research funding)
1986	Declined Berol Prize for best PhD Thesis in Sweden within the field of Surface and Colloid Chemistry. First prize to be awarded
1984	Royal Physiographic Society's Prize for best PhD Thesis in Chemistry at Lund University during the period 1981 - 84
1982	Postdoctoral Fellowship, Swedish Research Council
1977	University of California Reciprocity Fellowship

* Swedish Research Council - Natural and Engineering Sciences

Ten selected publications*

- *Cell water dynamics on multiple time scales*
E. Persson & B. Halle
Proc Natl Acad Sci USA **105** (17): 6266–6271 (2008) 44 citations
- *Molecular origin of time-dependent fluorescence shifts in proteins*
L. Nilsson & B. Halle
Proc Natl Acad Sci USA **102** (39): 13867–13872 (2005) 83 citations
- *Dynamics of protein and peptide hydration*
K. Modig, E. Liepinsh, G. Otting & B. Halle
J Am Chem Soc **126** (1): 102–114 (2004) 107 citations
- *Temperature-dependent hydrogen-bond geometry in liquid water*
K. Modig, B. G. Pfrommer & B. Halle
Phys Rev Lett **90** (7): 075502–075504pp (2003) 61 citations
- *Flexibility and packing in proteins*
B. Halle
Proc Natl Acad Sci USA **99** (3): 1274–1279 (2002) 107 citations
- *Sequence-specific binding of counterions to B-DNA*
V. P. Denisov & B. Halle
Proc Natl Acad Sci USA **97** (2): 629–633 (2001) 101 citations
- *Hydration of denatured and molten globule proteins*
V. P. Denisov, B. H. Jonsson & B. Halle
Nature Struct Biol **6** (3): 253–260 (1999) 152 citations
- *Using buried water molecules to explore the energy landscape of proteins*
V. P. Denisov, J. Peters, H. D. Hörlein & B. Halle
Nature Struct Biol **3** (6): 505–509 (1996) 123 citations
- *Protein hydration dynamics in aqueous solution*
V. P. Denisov & B. Halle
Faraday Discuss **103**: 295–311 (1996) 181 citations
- *Interpretation of magnetic resonance data from water nuclei in heterogeneous systems*
B. Halle & H. Wennerström
J Chem Phys **75** (4): 1928–1943 (1981) 477 citations

* citation counts from ISI, 24 March 2012

Original results published in peer-reviewed international journals

- 132 *Hydration dynamics of a halophilic protein in folded and unfolded states*
J. Qvist, G. Ortega, X. Tadeo, O. Millet & B. Halle
J Phys Chem B **116** (10): 3436–3444 (2012)
<http://dx.doi.org/10.1021/jp3000569>
- 131 *Structural dynamics of supercooled water from quasielastic neutron scattering and molecular simulations*
J. Qvist, H. Schober & B. Halle
J Chem Phys **134**, 144508:1–20 (2011)
<http://dx.doi.org/10.1063/1.3578472>
- 130 *High water mobility on the ice-binding surface of a hyperactive antifreeze protein*
K. Modig, J. Qvist, C. B. Marshall, P. L. Davies & B. Halle
Phys Chem Chem Phys **12** (35): 10189–10197 (2010)
<http://dx.doi.org/10.1039/C002970J>
- 129 *Mechanism of ^1H – ^{14}N cross-relaxation in immobilized proteins*
E. P. Sunde & B. Halle
J Magn Reson **203**, 257–273 (2010)
<http://dx.doi.org/10.1016/j.jmr.2010.01.008>
- 128 *The physical state of water in bacterial spores*
E. P. Sunde, L. Hederstedt, P. Setlow & B. Halle
Proc Natl Acad Sci USA **106** (46): 19334–19339 (2009)
<http://dx.doi.org/10.1073/pnas.0908712106>
- 127 *Slow internal protein dynamics from water ^1H magnetic relaxation dispersion*
E. P. Sunde & B. Halle
J Am Chem Soc **131** (51): 18214–18215 (2009)
<http://dx.doi.org/10.1021/ja908144y>
- 126 *The physical basis of model-free analysis of NMR relaxation data from proteins and complex fluids*
B. Halle
J Chem Phys **131** (22): 224507: 1–22 (2009)
<http://dx.doi.org/10.1063/1.3269991>
- 125 *Does the dynamic Stokes shift report on slow protein hydration dynamics?*
B. Halle & L. Nilsson
J Phys Chem B **113** (24): 8210–8213 (2009)
<http://dx.doi.org/10.1021/jp9027589>
- 124 *Protein cold denaturation as seen from the solvent*
M. Davidovic, C. Mattea, J. Qvist & B. Halle
J Am Chem Soc **131** (3): 1025–1036 (2009)
<http://dx.doi.org/10.1021/ja8056419>

- 123 *Internal sodium ions and water molecules in guanine quadruplexes: Magnetic relaxation dispersion studies of $[d(G_3T_4G_3)]_2$ and $[d(G_4T_4G_4)]_2$*
K. Snoussi & B. Halle
Biochemistry **47** (46): 12219–12229 (2008)
<http://dx.doi.org/10.1021/bi801657s>
- 122 *Thermal signature of hydrophobic hydration dynamics*
J. Qvist & B. Halle
J Am Chem Soc **130** (31): 10345–10353 (2008)
<http://dx.doi.org/10.1021/ja802668w>
- 121 *A dry ligand-binding cavity in a solvated protein*
J. Qvist, M. Davidovic, D. Hamelberg & B. Halle
Proc Natl Acad Sci USA **105** (17): 6296–6301 (2008)
<http://dx.doi.org/10.1073/pnas.0709844105>
- 120 *Nanosecond to microsecond protein dynamics probed by magnetic relaxation dispersion of buried water molecules*
E. Persson & B. Halle
J Am Chem Soc **130** (5): 1774–1787 (2008)
<http://dx.doi.org/10.1021/ja0775873>
- 119 *Cell water dynamics on multiple time scales*
E. Persson & B. Halle
Proc Natl Acad Sci USA **105** (17): 6266–6271 (2008)
<http://dx.doi.org/10.1073/pnas.0709585105>
- 118 *Dynamics at the protein-water interface from ^{17}O spin relaxation in deeply supercooled solutions*
C. Mattea, J. Qvist & B. Halle
Biophys J **95** (6): 2951–2963 (2008)
<http://dx.doi.org/10.1529/biophysj.108.135194>
- 117 *Internal water molecules and magnetic relaxation in agarose gels*
F. Vaca Chavez, E. Persson & B. Halle
J Am Chem Soc **128** (14): 4902–4910 (2006)
<http://dx.doi.org/10.1021/ja058837n>
- 116 *Hydrogen exchange and hydration dynamics in gelatin gels*
F. Vaca Chavez, E. Hellstrand & B. Halle
J Phys Chem B **110** (43): 21551–21559 (2006)
<http://dx.doi.org/10.1021/jp057567s>
- 115 *Molecular basis of water proton relaxation in gels and tissue*
F. Vaca Chavez & B. Halle
Magn Reson Med **56** (1): 73–81 (2006)
<http://dx.doi.org/10.1002/mrm.20912>

- 114 *Molecular theory of field-dependent proton spin-lattice relaxation in tissue*
B. Halle
Magn Reson Med **56** (1): 60–72 (2006)
<http://dx.doi.org/10.1002/mrm.20919>
- 113 *Protein self-association induced by macromolecular crowding: A quantitative analysis by magnetic relaxation dispersion*
K. Snoussi & B. Halle
Biophys J **88** (4): 2855–2866 (2005)
<http://dx.doi.org/10.1529/biophysj.104.055871>
- 112 *Molecular origin of time-dependent fluorescence shifts in proteins*
L. Nilsson & B. Halle
Proc Natl Acad Sci USA **102** (39): 13867–13872 (2005)
<http://dx.doi.org/10.1073/pnas.0504181102>
- 111 *Dynamics of protein and peptide hydration*
K. Modig, E. Liepinsh, G. Otting & B. Halle
J Am Chem Soc **126** (1): 102–114 (2004)
<http://dx.doi.org/10.1021/ja038325d>
- 110 *Biomolecular cryocrystallography: Structural changes during flash-cooling*
B. Halle
Proc Natl Acad Sci USA **101** (14): 4793–4798 (2004)
<http://dx.doi.org/10.1073/pnas.0308315101>
- 109 *Stabilization of internal charges in a protein: Water penetration or conformational change?*
V. P. Denisov, J. L. Schlessman, B. Garcia-Moreno & B. Halle
Biophys J **87** (6): 3982–3994 (2004)
<http://dx.doi.org/10.1529/biophysj.104.048454>
- 108 *Accelerated exchange of a buried water molecule in selectively disulfide-reduced bovine pancreatic trypsin inhibitor*
V. P. Denisov, J. Peters, H. D. Hörlein & B. Halle
Biochemistry **43** (38): 12020–12027 (2004)
<http://dx.doi.org/10.1021/bi0492049>
- 107 *Competitive Na⁺ and Rb⁺ binding in the minor groove of DNA*
F. Cesare Marincola, V. P. Denisov & B. Halle
J Am Chem Soc **126** (21): 6739–6750 (2004)
<http://dx.doi.org/10.1021/ja049930z>
- 106 *Water dynamics in the large cavity of three lipid-binding proteins monitored by ¹⁷O magnetic relaxation dispersion*
K. Modig, M. Rademacher, C. Lücke & B. Halle
J Mol Biol **332** (4): 965–977 (2003)
[http://dx.doi.org/10.1016/S0022-2836\(03\)00968-9](http://dx.doi.org/10.1016/S0022-2836(03)00968-9)

- 105 *Temperature-dependent hydrogen-bond geometry in liquid water*
K. Modig, B. G. Pfrommer & B. Halle
Phys Rev Lett **90** (7): 075502–075504pp (2003)
<http://dx.doi.org/10.1103/PhysRevLett.90.075502>
- 104 *Water and urea interactions with the native and unfolded forms of a β -barrel protein*
K. Modig, E. Kurian, F. G. Prendergast & B. Halle
Protein Sci **12** (12): 2768–2781 (2003)
<http://www3.interscience.wiley.com/journal/121602044/abstract>
- 103 *Trifluoroethanol-induced $\beta \rightarrow \alpha$ transition in β -lactoglobulin: Hydration and cosolvent binding studied by ^2H , ^{17}O , and ^{19}F magnetic relaxation dispersion*
S. Kumar, K. Modig & B. Halle
Biochemistry **42** (46): 13708–13716 (2003)
<http://dx.doi.org/10.1021/bi035330l>
- 102 *Biomolecular hydration: From water dynamics to hydrodynamics*
B. Halle & M. Davidovic
Proc Natl Acad Sci USA **100** (21): 12135–12140 (2003)
<http://dx.doi.org/10.1073/pnas.2033320100>
- 101 *Cross-relaxation between macromolecular and solvent spins: The role of long-range dipole couplings*
B. Halle
J Chem Phys **119** (23): 12372–12385 (2003)
<http://dx.doi.org/10.1063/1.1625632>
- 100 *Protein self-association in solution: The bovine pancreatic trypsin inhibitor decamer*
M. Gottschalk, K. Venu & B. Halle
Biophys J **84** (6): 3941–3958 (2003)
[http://dx.doi.org/10.1016/S0006-3495\(03\)75122-4](http://dx.doi.org/10.1016/S0006-3495(03)75122-4)
- 99 *Protein self-association in solution: The bovine β -lactoglobulin dimer and octamer*
M. Gottschalk, H. Nilsson, H. Roos & B. Halle
Protein Sci **12** (11): 2404–2411 (2003)
<http://www3.interscience.wiley.com/journal/121602013/abstract>
- 98 *Self-association of lysozyme as seen by magnetic relaxation dispersion*
M. Gottschalk & B. Halle
J Phys Chem B **107** (31): 7914–7922 (2003)
<http://dx.doi.org/10.1021/jp034527k>
- 97 *Proton magnetic shielding tensor in liquid water*
K. Modig & B. Halle
J Am Chem Soc **124** (40): 12031–12041 (2002)
<http://dx.doi.org/10.1021/ja026981s>

- 96 *Flexibility and packing in proteins*
B. Halle
Proc Natl Acad Sci USA **99** (3): 1274–1279 (2002)
<http://dx.doi.org/10.1073/pnas.032522499>
- 95 *Hydrogen exchange rates in proteins from water ¹H transverse magnetic relaxation*
V. P. Denisov & B. Halle
J Am Chem Soc **124** (35): 10264–10265 (2002)
<http://dx.doi.org/10.1021/ja027101c>
- 94 *Microsecond exchange of internal water molecules in bacteriorhodopsin*
M. Gottschalk, N. A. Dencher & B. Halle
J Mol Biol **311** (3): 605–621 (2001)
<http://dx.doi.org/10.1006/jmbi.2001.4895>
- 93 *Sequence-specific binding of counterions to B-DNA*
V. P. Denisov & B. Halle
Proc Natl Acad Sci USA **97** (2): 629–633 (2000)
<http://www.pnas.org/content/97/2/629.abstract?sid=72200c67-35b7-43e8-9ab3-0e8d64352689>
- 92 *Water molecules in the binding cavity of intestinal fatty acid binding protein: Dynamic characterization by water ¹⁷O and ²H magnetic relaxation dispersion*
S. Wiesner, E. Kurian, F. G. Prendergast & B. Halle
J Mol Biol **286** (1): 233–246 (1999)
<http://dx.doi.org/10.1006/jmbi.1998.2490>
- 91 *Orientalional order and dynamics of hydration water in a single crystal of bovine pancreatic trypsin inhibitor*
K. Venu, L. A. Svensson & B. Halle
Biophys J **77** (2): 1074–1085 (1999)
[http://dx.doi.org/10.1016/S0006-3495\(99\)76957-2](http://dx.doi.org/10.1016/S0006-3495(99)76957-2)
- 90 *Deuteron relaxation dispersion in aqueous colloidal silica*
P. Roose, H. Bauwin & B. Halle
J Phys Chem B **103** (25): 5167–5174 (1999)
<http://dx.doi.org/10.1021/jp984277l>
- 89 *Dissection of the structural and functional role of a conserved hydration site in RNase T1*
U. Langhorst, R. Loris, V. P. Denisov, J. Doumen, P. Roose, D. Maes, B. Halle & J. Steyaert
Protein Sci **8** (4): 722–730 (1999)
<http://www3.interscience.wiley.com/journal/121601217/abstract>
- 88 *Hydration of denatured and molten globule proteins*
V. P. Denisov, B. H. Jonsson & B. Halle
Nat Struct Biol **6** (3): 253–260 (1999)
<http://dx.doi.org/10.1038/6692>

- 87 *Dynamics of functional water in the active site of native carbonic anhydrase from ^{17}O magnetic relaxation dispersion*
V. P. Denisov, B. H. Jonsson & B. Halle
J Am Chem Soc **121** (10): 2327–2328 (1999)
<http://dx.doi.org/10.1021/ja983930f>
- 86 *Water molecules in DNA recognition. Hydration lifetimes of trp operator DNA in solution measured by NMR spectroscopy*
M. Sunnerhagen, V. P. Denisov, K. Venu, A. M. J. J. Bonvin, J. Carey, B. Halle & G. Otting
J Mol Biol **282** (4): 847–858 (1998)
<http://dx.doi.org/10.1006/jmbi.1998.2033>
- 85 *Minor groove hydration of DNA in solution: Dependence on base composition and sequence*
H. Jóhannesson & B. Halle
J Am Chem Soc **120** (28): 6859–6870 (1998)
<http://dx.doi.org/10.1021/ja974316r>
- 84 *Model-free analysis of stretched relaxation dispersions*
B. Halle, H. Jóhannesson & K. Venu
J Magn Reson **135** (1): 1–13 (1998)
<http://dx.doi.org/10.1006/jmre.1998.1534>
- 83 *Thermal denaturation of ribonuclease A characterized by water ^{17}O and ^2H magnetic relaxation dispersion*
V. P. Denisov & B. Halle
Biochemistry **37** (26): 9595–9604 (1998)
<http://dx.doi.org/10.1021/bi980442b>
- 82 *Water ^1H magnetic relaxation dispersion in protein solutions. A quantitative assessment of internal hydration, proton exchange, and cross-relaxation*
K. Venu, V. P. Denisov & B. Halle
J Am Chem Soc **119** (13): 3122–3134 (1997)
<http://dx.doi.org/10.1021/ja963611t>
- 81 *Fluid membrane interactions probed by nuclear spin relaxation*
P. O. Quist & B. Halle
Phys Rev Lett **78** (19): 3689–3692 (1997)
<http://dx.doi.org/10.1103/PhysRevLett.78.3689>
- 80 *NMR identification of hydrophobic cavities with low water occupancies in protein structures using small gas molecules*
G. Otting, E. Liepinsh, B. Halle & U. Frey
Nat Struct Biol **4** (5): 396–404 (1997)
<http://dx.doi.org/10.1038/nsb0597-396>
- 79 *Dimethyl sulfoxide binding to globular proteins: A nuclear magnetic relaxation dispersion study*
H. Jóhannesson, V. P. Denisov & B. Halle
Protein Sci **6** (8): 1756–1763 (1997)
<http://www3.interscience.wiley.com/journal/121600652/abstract>

- 78 *Diffusion in a fluctuating random geometry*
B. Halle & S. Gustafsson
Phys Rev E **55** (1): 680–686 (1997)
<http://dx.doi.org/10.1103/PhysRevE.55.680>
- 77 *Orientational correlations and spin relaxation in lamellar fluid membrane phases*
B. Halle & S. Gustafsson
Phys Rev E **56** (1): 690–707 (1997)
<http://dx.doi.org/10.1103/PhysRevE.56.690>
- 76 *Diffusion on a flexible surface*
S. Gustafsson & B. Halle
J Chem Phys **106** (5): 1880–1887 (1997)
<http://dx.doi.org/10.1063/1.473326>
- 75 *Spin relaxation by collective director fluctuations and molecular diffusion in lamellar phases. Continuum theory of relaxation anisotropy and dispersion*
S. Gustafsson & B. Halle
J Chem Phys **106** (22): 9337–9352 (1997)
<http://dx.doi.org/10.1063/1.474003>
- 74 *Spin relaxation by diffusion on biaxial rods*
S. Gustafsson & B. Halle
J Chem Phys **107** (5): 1460–1469 (1997)
<http://dx.doi.org/10.1063/1.474499>
- 73 *Orientational disorder and entropy of water in protein cavities*
V. P. Denisov, K. Venu, J. Peters, H. D. Hörlein & B. Halle
J Phys Chem B **101** (45): 9380–9389 (1997)
<http://dx.doi.org/10.1021/jp9712213>
- 72 *Kinetics of DNA hydration*
V. P. Denisov, G. Carlström, K. Venu & B. Halle
J Mol Biol **268** (1): 118–136 (1997)
<http://dx.doi.org/10.1006/jmbi.1996.0862>
- 71 *Solvent diffusion in ordered macrofluids: A stochastic simulation study of the obstruction effect*
H. Jóhannesson & B. Halle
J Chem Phys **104** (17): 6807–6817 (1996)
<http://dx.doi.org/10.1063/1.471347>
- 70 *Orientational order and micelle size in the nematic phase of the cesium pentadecafluorooctanoate-water system from the anisotropic self-diffusion of water*
H. Jóhannesson, I. Furó & B. Halle
Phys Rev E **53** (5): 4904–4917 (1996)
<http://dx.doi.org/10.1103/PhysRevE.53.4904>

- 69 *Spin dynamics of exchanging quadrupolar nuclei in locally anisotropic systems*
B. Halle
Prog NMR Spectrosc **28** (2): 137–159 (1996)
[http://dx.doi.org/10.1016/0079-6565\(95\)01022-X](http://dx.doi.org/10.1016/0079-6565(95)01022-X)
- 68 *Using buried water molecules to explore the energy landscape of proteins*
V. P. Denisov, J. Peters, H. D. Hörlein & B. Halle
Nat Struct Biol **3** (6): 505–509 (1996)
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